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Abstract Submission

Submission-807

Topic : / Computer-aided Engineering / Process Systems Engineering / ECCE10 / Process modelling and simulation

A SYSTEMATIC MODELLING FRAMEWORK FOR PHASE TRANSFER CATALYST SYSTEMS

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Submit your abstract below (400 words): Catalytic two-phase reaction systems have been known for many years, yet there are no systematic model-based methods for their design and/or analysis. The reaction system contains two immiscible liquid phases, with heterogeneous phase transfer catalyst (PTC) transferring active ions from one phase to the other for converting the reactant to the desired product, and in the process generating the inactive ion. Therefore, this type of reacting systems is receiving increasing attention as a novel organic synthesis option. Moreover application of the PTC system allows flexible and easier operation, higher production yield, and eliminates hazardous or expensive solvents, although, not eliminating the use of solvents. Modelling of PTC systems is a formidable challenge due to the complexity of the involved phenomena and therefore, the need for appropriate thermodynamic models capable of describing the phase behaviour of systems involving water, organic solvents, inorganic salts, and the PTC; the reaction and mass-transfer mechanisms involved in these systems; as well as, the lack of experimental data.

The aim of this work is to develop a modelling framework that requires minimum amount of experimental data to predict the behaviour of PTC systems. In the framework, the models are formulated according to a systematic step by step procedure. A new group contribution based thermodynamic model for electrolyte systems (e-KT-UNIFAC) and segment based thermodynamics model (e-NRTL-SAC and NRTL-SAC) have been developed and implemented within the framework. The objective is to broaden the application range of the process model and to reduce the number of experimental data required.

Three types of models: equilibrium, conversion, and kinetic based, for describing the PTC system under different scenarios will be presented. A case study demonstrating the application of the models for various PTC-involving reactions will be highlighted. Analysis of the results verifying and validating the effects of solvents and the PTCs selection will be presented.

Type of presentation :: Oral

Highlight 1: A modelling framework for predicting the behaviour of PTC systems

Highlight 2: A new group contribution based thermodynamic model for electrolyte systems (e-KT-UNIFAC)

Highlight 3: A case study demonstrating the application of the models for various scenarios



Keywords: Catalysis, Phase equilibrium , Process modelling, Process system engineering, Simulation